Ethylene oxide 75-21-8 | DTXSID0020600

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 2.08

Global applicability domain: Inside

Local applicability domain index: 9.42e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

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Acetonitrile
Measured: 2.31
Predicted: 1.96

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Methyl formate Measured: 1.75 Predicted: 1.78 Image not found

Propane
Measured: 0.97
Predicted: 1.60

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Nitroethane Measured: 2.88 Predicted: 2.25 Image not found

Nitromethane Measured: 2.53 Predicted: 1.63